

# Application Of The Direct Simulation Monte Carlo Method To Modeling Of Microfluidics

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## ABSTRACT

For mathematical modeling of microfluidics it is necessary to calculate a rarefied gas flow through micropumps, microvalves and other elements with high accuracy. Since the size of microfluidics is close to the molecular mean free path, the modeling cannot be performed on the basis of the continuum mechanics equations, but the gas rarefaction must be taken into account. In the paper one of the methods of rarefied gas dynamics is demonstrated by means of its application to an internal gas flow. The problem is solved in wide range of the Knudsen number that shows a significant difference of the solution for different degrees of the gas rarefaction.

**Keywords:** Microfluidics, Rarefied Gas, Direct Simulation

## 1 INTRODUCTION

The gas rarefaction is characterized by the Knudsen number defined as

$$Kn = \lambda/a, \quad (1)$$

where  $\lambda$  is the molecular mean free path, and  $a$  is a characteristic size of the gas flow. In the previous paper [1] a consideration of the gas rarefaction by means of the slip coefficients was described. However, this method is restricted by the small Knudsen numbers, i.e. near the hydrodynamic regime of the gas flow. Since the size of microfluidics constantly decreases, methods applicable at arbitrary Knudsen numbers should be used for their numerical modeling.

Nowadays, the Direct Simulation Monte Carlo (DSMC) method [2] becomes a powerful tool to calculate the gas flow at any gas rarefaction. The main idea of the method is as follows: The region of the gas flow is divided into a network of cells. The dimensions of the cells must be such that the change in flow properties across each cell is small. The time is advanced in discrete steps of magnitude  $\Delta t$ , such that  $\Delta t$  is small compared with the mean time between two successive collisions.

The molecular motion and intermolecular collision are uncoupled over the small time interval  $\Delta t$  by the repetition of the following procedure:

i) the molecules are moved through the distance determined by their velocities and  $\Delta t$ . If the trajectory passes the boundary a simulation of the gas-surface interaction is performed in according to a given law. New molecules are generated at boundaries across which there is an inward flux.

ii) A representative number of collisions appropriate to  $\Delta t$  and number of molecules in the cell is computed. The pre-collision velocities of the molecules involved in the collision are replaced by the post-collision values in accordance with a given law of the intermolecular interaction.

After a sufficient number of the repetitions the macroscopic characteristics (mass flow rate, heat flux, pressure and temperature distributions, etc.) are calculated.

The aim of the present work is to applying the DSMC method for an internal rarefied gas flow that is realized in microfluidics, namely the gas flow through an orifice. The solution of this problem is determined by the two main parameters: the Knudsen number (1) and the pressure ratio  $P_0/P_1$ . Here  $P_0$  is the upflow pressure,  $P_1$  is the downflow pressure. We assume  $\lambda$  to be related to the up flow pressure  $P_0$  and  $a$  to be the orifice radius.

In spite of the great practical importance till now this problem has not been investigated profoundly. As was noted in the review [3] a number of papers [4]–[7] offered asymptotic formulas for the mass flow rate near the free-molecular regime ( $Kn \rightarrow \infty$ ) in case of outflow into vacuum ( $P_0/P_1 = \infty$ ). But there is no agreement between them and the range of their validity is very small. Some numerical data for intermediate Knudsen numbers and for the infinite pressure ratio  $P_0/P_1$  can be found in the work by Shakhov [8]. But the presentation of the data is very poor. In case of the small pressure difference, i.e.  $|P_0 - P_1| \ll P_0$ , the problem can be solved analytically in the hydrodynamic regime ( $Kn \ll 1$ ). The corresponding results are given in the works by Roscoe [9] and by Hasimoto [10]. Thus, one can see that the theoretical results on the orifice flow is restricted by the small ranges of the Knudsen number  $Kn$  and of the pressure ratio  $P_0/P_1$ .

Experimental results on the mass flow rate through an orifice in case of outflow into vacuum ( $P_0/P_1 = \infty$ ) are presented in the papers by Liepmann [4], by Fujimoto and Usami [11], and by Barashkin *et al.* [12], [13].

Experimental data for some intermediate values of the pressure ratio  $P_0/P_1$  but for a restricted range of the Knudsen number are given in the paper by Sreekanth [14]. The works by Borisov *et al.* [15] and by Porodnov *et al.* [16] provide the experimental results for the small pressure difference, i.e.  $|P_0 - P_1| \ll P_0$ , in a wide range of the Knudsen number. So, the experimental material on the orifice flow is also poor.

## 2 Statement of the problem

Consider an orifice in an infinitely thin partition that separates two semi-infinite reservoirs. One of them contains a monoatomic gas at a temperature  $T_0$  and at a pressures  $P_0$ . The other container is maintained under a high vacuum so it can be considered that  $P_1 = 0$ . The schematic diagram of the flow is given in Fig.1,  $x$  is the axis of the orifice and  $r$  is the radial coordinate.

We are going to calculate the mass flow rate and the flow field as a function of the rarefaction parameter  $\delta$  defined as

$$\delta = \frac{\sqrt{\pi}}{2} \frac{1}{\text{Kn}} = \frac{\sqrt{\pi}}{2} \frac{a}{\lambda}, \quad (2)$$

where the mean free path  $\lambda$  is related to the pressure  $P_0$  and the temperature  $T_0$  as

$$\lambda = \frac{\mu(T_0)}{P_0} \left( \frac{\pi k T_0}{2m} \right)^{1/2}.$$

Here,  $\mu(T_0)$  is the viscosity at the temperature  $T_0$ ,  $m$  is the mass of a gaseous particle and  $k$  is the Boltzmann constant.

The numerical results will be given in terms of the reduced mass flow rate defined as

$$W = \frac{\dot{M}}{\dot{M}_0}, \quad (3)$$

where  $\dot{M}$  is the dimension mass flow rate and  $\dot{M}_0$  is the mass flow rate in the free molecular regime flow, which reads

$$\dot{M}_0 = a^2 P_0 \left( \frac{\pi m}{2kT_0} \right)^{1/2}. \quad (4)$$

## 3 Method of solution

The problem was solved by the direct simulation Monte Carlo method [2]. It was assumed the diffuse gas-surface interaction and the hard sphere molecular model. The region for the flow simulation has the form of two cylinders. The cylinders have the radii  $R_0$  and  $R_1$  and the lengths  $L_0$  and  $L_1$  in the upflow and downflow containers, respectively. The sizes of the region were as follows:  $L_0 = R_0 = 8a$  and  $L_1 = R_1 = 4a$ . The numerical grid was regular with the cell size equal to  $\Delta x = \Delta r = a/8$ . The time increment was 0.01 of the mean

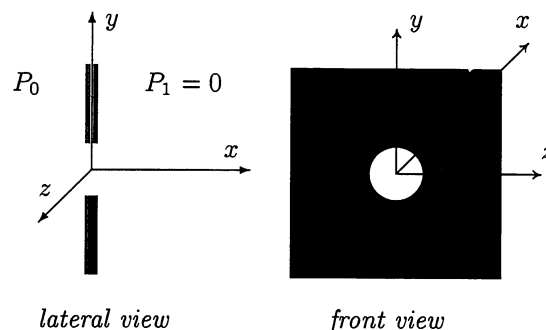


Figure 1: Schematic diagram and coordinates

free time. The number of simulated molecules fluctuate during the calculation. It was maintained about the value  $10^6$ .

To simulate the collision the so-called NTC method, see Ref. [2], p.219, was used. In every cell the number of selected pairs was calculates as

$$\frac{1}{2} N_c \overline{N}_c F_N \sigma c_{r,max} \frac{\Delta t}{V_c},$$

where  $N_c$  is the number of particles in the cell,  $\overline{N}_c$  is the average value of  $N_c$ ,  $F_N$  is the number of real molecules that each simulated particle represents,  $\sigma$  is the diameter of particle,  $c_{r,max}$  is the maximum relative velocity,  $\Delta t$  is the time increment, and  $V_c$  is the volume of the cell.

In every time step the number of particle passed through the orifice from the upflow container to the downflow one and the number of particles passed the orifice in the opposite direction were counted. The mass flow rate was calculated based on the average numbers of particles passed through the orifice during  $10^5$  time steps that correspond to the time interval equal to  $10^3$  mean free times.

## 4 Results and discussions

The calculations were carried out for the rarefaction parameter range  $0.05 \leq \delta \leq 100$ . For the values of  $\delta$  smaller than 0.05 the mass flow rate  $W$  does not differ from the unity within 1%. In the range  $20 \leq \delta \leq 100$  it was observed the variation of the mass flow rate within 0.5%. So, a significant variation of the mass flow rate occurs in the range  $0.1 \leq \delta \leq 20$ .

The reduced mass flow rate  $W$  is presented in Fig. 2 as a function of the rarefaction parameter  $\delta$ . One can see that the quantity  $W$  varies in the range from 1 to 1.5. Then, beginning from  $\delta = 20$  the mass flow rate  $W$  is practically constant by increasing the rarefaction parameter  $\delta$ .

Fujimoto and Usami [11] measured the mass flow rate through short tubes. The length-to-radius ratio of the

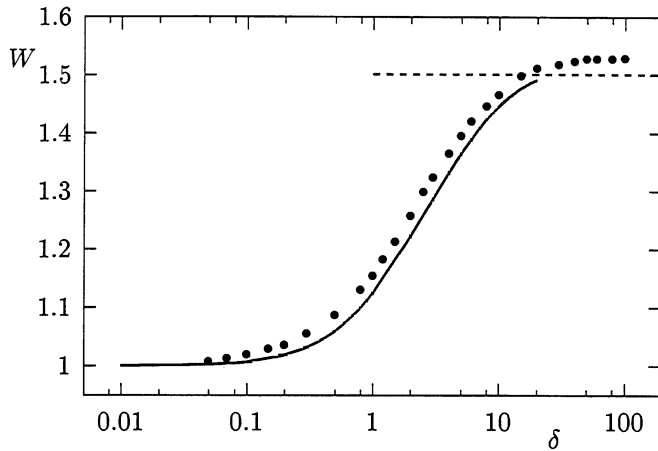


Figure 2: Mass flow rate  $W$  vs  $\delta$ : points - present work, solid line - empirical formulae [11], dashed line - experiment at  $\delta \rightarrow \infty$  [12]

shortest tube was  $l/a = 0.025$  that can be considered as an orifice. They offered an empirical equation of the mass flow rate based on the experimental data for the interval  $0.025 \leq l/a \leq 12.7$  and for the large pressure ratio  $P_0/P_1 > 0.01$  that can be considered as an outflow into vacuum. If one extrapolates their empirical equation for the orifice ( $l/a = 0$ ), one obtains

$$W = 1 + \frac{0.4733 + 0.6005/\sqrt{\delta}}{1 + 4.559/\delta + 3.094/\delta^2}. \quad (5)$$

This formulae is presented by the solid line in Fig. 2. One can see that in the range  $0 \leq \delta \leq 20$  the empirical formulae and the numerical simulation results are in a good agreement. The systematic understanding of the empirical formulae is explained by the fact that the shortest tube in the experiments [11] was of  $l/a = 0.025$  that decreases the mass flow for few percents. Moreover, the downflow pressure that always exists in experiment also slightly decreases the mass flow rate.

Barashkin *et al.* [12] also measured the mass flow through an orifice. In the hydrodynamic regime ( $\delta \rightarrow \infty$ ) they reported the value  $W = 1.501$  for the argon gas. This result is given in Fig. 2 by the dashed line. One can see that the numerical results in the range  $20 \leq \delta \leq 100$  slightly overstate the experimental data by Barashkin *et al.* [12]. This small disagreement can be explained by analyzing the results by Fujimoto and Usami [11]. They show that in the interval of the rarefaction parameter  $\delta$  from 50 to 1000 the mass flow rate  $W$  has a small decrease. So, it is possible that the flow rate  $W$  reported in the work [12] are based on high values of  $\delta$ , i.e. about 1000. To obtain theoretically the limit value of the mass flow rate a new simulation should be carried out for larger values of  $\delta$  that will require great computational efforts.

The number density distribution  $n/n_0$  is given in Fig.

3 for the three values of the rarefaction parameter  $\delta = 0.1$ ; 1.0 and 10. Here,  $n_0 = P_0/kT_0$ . One can see that near the free molecular regime ( $\delta = 0.1$ ) the density field is practically symmetric, i.e.

$$n(x, r) = n_0 - n(-x, r). \quad (6)$$

It is easy to prove that in the free molecular regime ( $\delta = 0$ ) the density field satisfies the relation (6) exactly. By increasing the rarefaction parameter  $\delta$  the contour lines dislocate to the downflow container and at  $\delta = 10$  the density is almost uniform in the upflow container.

The mass flux vector

$$\mathbf{J} = n\mathbf{u} \quad (7)$$

is given in Fig. 4. Here,  $\mathbf{u}$  is the bulk velocity. This field changes quantitatively by increasing the rarefaction parameter  $\delta$ , i.e. the mass flux increases. But the qualitative variation is small.

## 5 Conclusion

The mass flow rate of rarefied gas through a thin orifice has been calculated by the direct simulation Monte Carlo method in the range of the rarefaction parameter from 0.005 to 100 under the assumption of a large pressure ratio. It has been found that in this range the reduced flow rate varies from 1 to 1.5. Outside of this range the variation of the mass flow rate is very small, i.e. within 1%. The numerical data are in a good agreement with the experimental data available in open literature.

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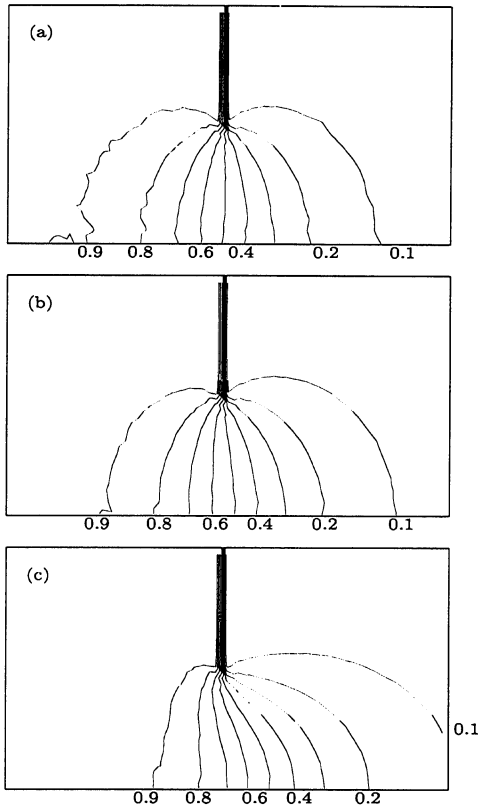


Figure 3: Number density distribution  $n/n_0$ : (a) -  $\delta = 0.1$ ; (b) -  $\delta = 1.0$ ; (c) -  $\delta = 10$ .

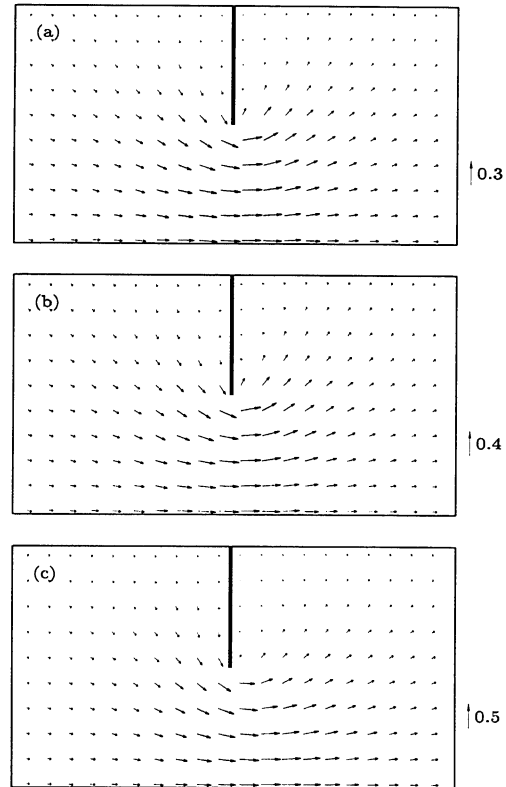


Figure 4: Mass flux vector  $\mathbf{J}$ : (a) -  $\delta = 0.1$ ; (b) -  $\delta = 1.0$ ; (c) -  $\delta = 10$ .

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